Los Alamos
NATIONAL LABORATORY
research note

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LA-UR-01-1655
Date: June 18, 2001

Release Notes for LAHET Code System with LAHET^{TM} Version 3.16

Summary

The release of LAHET^{TM} Version 3.16 as a "friendly-user" version of LAHET3 is described. A description of the input for the new version is given, as are instructions for interfacing with MCNP and MCNPX.

I. Introduction

The release of LAHET^{TM} Version 3.0[1] was the first "friendly-user" version of LAHET3 provided for internal use at Los Alamos National Laboratory and represented a significant advance from previously released versions of LAHET[2, 3]. The physics modules from LAHET3.0 were those which were supplied for the initial versions of MCNPX^{TM} [4], the LAHET/MCNP code merger.

New features included in LAHET3.0 were the high-energy generator from FLUKA89[5], the gamma de-excitation code PHT[2] as an inline module, and a simplified interface to MCNP^{TM} [6]. The user input to LAHET3.0 was greatly modified.

New features added in LAHET3.16 for this release include:

1. the adaptation of the FLUKA96[7] high-energy generator, replacing the older version in LAHET3.0;
2. the implementation of a procedure to provide defined reaction and elastic scattering cross sections for all particles in LAHET and, in the absence of nuclear data libraries, in MCNPX[8] (see Table 1);
3. the development of a new atomic mass data base and the code to access it for all the physics packages shared by LAHET and MCNPX[8];
4. the construction of a stopping power generator that is much improved over the original method used in earlier LAHET versions for the transport of all particles with mass greater than or equal to the muon[8];

5. the option for primary beam transport with attenuation but without executing nonelastic reactions[9].

The HTAPE3 and XSEX3 codes continue to play the same role in the Lahet Code System as did HTAPE and XSEX for earlier versions; for use of the codes, the user is referred to the original documentation[2, 3] and to reference[10]. However, XSEX3 now includes the option to write an output file in the format of an MCNP MCTAL file, for the purpose of plotting calculated cross sections (see section VIII.)

II. Overview of LAHET Input

The full structure of the LAHET input file (conventionally named INH) is as follows.

- **LAHET Control Records**, in free-form input.
- **MCNP Geometry Records**.
- **Other MCNP-type Records**, including LAHET physics options.
- **Source Description Records**.

The input file structure for Version 3 is **not** backward-compatible with any previous version of LAHET. The restructuring of input is part of the effort to effect the merger of LAHET and MCNP.

III. LAHET Control Records

The LAHET input records are as follows.

Record 1 First line of title.

Record 2 Second line of title.

Record 3 Format (Z12) with one item. A blank record must be supplied if only the default is desired.

RANDOM A 12-digit hexadecimal number for the starting random number; *the default is 1123456789AB.*

Record 4 List-directed with 8 data items.

MAXCAS The number of cascades in one batch. The *default is 0;* MAXCAS = 0 will process input and halt execution.

MAXBCH The number of batches to run; the *default is 1* and *must be* > 0. Nothing in the LAHET Code System makes use of batched history file data; it is appropriate for use with a history file statistical editor that computes batch statistics.

MXMAT The number of different media in the problem, exclusive of voids. The *default is 0*, but MXMAT is not limited.

NOSKIP 0 ⇒ the next available random number is used to initiate a cascade;
> 0 ⇒ the random number is advanced 4297×NOSKIP each history.

The *default is 10.* Any value < 0 is an error condition. Using NOSKIP > 0 allows each history to start with a predetermined random number, allowing one to "inspect" a troublesome history in a subsequent run by using the JCASC parameter above. The purpose of using a large NOSKIP parameter is to prevent multiple use of the random number string between histories when many random numbers are generated per history.

NLIMIT The maximum number of low energy neutrons to put on any one neutron file; the *default is 10000000* and 0 takes the default.

LHIST The maximum length of any one history file in single precision words. The *default is* 2^{29} and 0 takes the default; the minimum is 2^{15}.

NBMX Length of particle bank in number of particles. Bank overflows are written to a scratch file. The *default is 256.*

JCASC Forces the calculation to start with history number JCASC in the sequence of random numbers defined by RANDOM. The *default is 1* and JCASC ≤ 0 takes the default. The use of JCASC is primarily a debugging tool; it allows one to start a run with a particular history which may have occurred in a previous run which one may wish to examine. It is applicable *only for NOSKIP ≥ 1.*

Record 5 List-directed with 6 data items.

NBERTP 1 ⇒ nucleon-pion transport only *(default)*;
0 ⇒ muon transport only;
-1 ⇒ nucleon-pion-muon transport.

Other values are an error condition. The file BERTIN is required for NBERTP = ±1.

MODEXS 0 ⇒ apply new cross section definition procedure *(default)*; otherwise, revert to method of all previous versions. The specific definitions used in LAHET3.16 are shown in Table 1 below; discussion of the methods is found in reference [11].

NEUTP 0 ⇒ do not write NEUTP;
1 ⇒ write photons and low energy neutrons to file NEUTP *(default)*;

Other values are an error condition.

NHSTP 1 ⇒ write history file HISTP *(default)*;
0 ⇒ do not write HISTP.

Other values are an error condition.

MXHIST Maximum number of history files to allow; the *default is 27* and zero defaults to 27. The absolute maximum number of history tapes is 27, with the naming

NCOL	record type
1	source
2	nuclear interaction (secondaries from cascade)
3	charged particle slowed to cutoff
4	escape from system
5	pseudo-collision
6	nuclear absorption (no secondaries from cascade)
7	internal boundary crossing
8	multiple scattering subtrajectory

Table 1: HISTP Record Types

sequence HISTP, HISTPA,...,HISTPZ. The run will terminate if MXHIST is exceeded. *NOTE:* the maximum number of files is reduced if any files in the naming sequence are present in the local file space.

IRECRD 0 $\Rightarrow$ use default record control to specify data to be put on history file;
1 $\Rightarrow$ read records 5a and 5b to control the contents of the history file.

The *default = 0*; all other values are an error condition. The default mode excludes only multiple scattering subtrajectory records (NCOL = 8) and nucleon pseudo-collision records; these are rarely used except for debugging purposes. The remaining records are those necessary for a complete energy balance. All particles which are transported are included on the history file.

Record 5a List-directed with 8 items (present only for IRECRD = 1).

KREC(I),I=1,8 0 $\Rightarrow$ write records for NCOL = I;
1 $\Rightarrow$ suppress records for NCOL = I.

The definition of the record types NCOL are given in Table 1.

Record 5b List-directed with (up to) 22 items (present only for IRECRD = 1).

KPART(I),I=1,22
0 $\Rightarrow$ write records for particle index I;
1 $\Rightarrow$ suppress records for particle index I.

A list of the particle indices is given in Table 2. Note that the π^0 and photon do not cause any HISTP records to be written, so that whether KPART(4) or KPART(12) is 1 or 0 is immaterial.

Index	Type	Particle	Source ?
1	0.	proton	Yes
2	1.	neutron	Yes
3	2.	π^+	Yes
4	3.	π^0	No
5	4.	π^-	Yes
6	5.	μ^+	Yes
7	6.	μ^-	Yes
8	7.	deuteron	Yes
9	8.	triton	Yes
10	9.	^{3}He	Yes
11	10.	alpha	Yes
12	11.	photon	No
13	12.	K^+	Yes
14	13.	K^0long	Yes
15	14.	K^0short	Yes
16	15.	K^-	Yes
17	16.	$\overline{p}$	Yes
18	17.	$\overline{n}$	Yes
19	18.	electron	No
20	19.	positron	No
21	20.	neutrino	No
22	21.	antineutrino	No

Table 2: Particle Type Identification

Record 6 List-directed with 3 items.

N1COL 2 $\Rightarrow$ allow source particle interactions only and do *not* track secondary particles;
1 $\Rightarrow$ compute cascade histories only through the second generation;
0 $\Rightarrow$ compute all generations *(default)*;
-1 $\Rightarrow$ compute nuclear interactions of source particles only.

Other values are an error condition. For N1COL = -1, transport and slowing-down are turned off. Only nuclear interaction records are written to HISTP (NCOL=2 and NCOL=6). The interaction occurs in the first material of the problem; any other material specified is not used in the problem. This option is useful in calculating cross sections using the XSEX3 code to process HISTP. When using this option, it may be desirable to set the total atom density in the material to 1.0 so that XSEX3 will produce cross sections directly in barns.

LISTXS 1 ⇒ print out a standard edit of reaction and elastic scattering cross sections to file XSTEST.OUT;
0 ⇒ no such printout *(default)*.

Other values are an error condition.

ISRFSR 1 ⇒ read surface source from file HISTIN;
0 ⇒ use default source or user-supplied source *(default)*.

Other values are an error condition.

Record 7 List-directed with 4 items, all floating point.

EMAX The maximum energy for particles in MeV. The *default is 3495 MeV* and 0 defaults to 3495 MeV. For the Bertini INC model there is no upper limit on EMAX, although the scaling law model used to extrapolate the Bertini model above 3.5 GeV gets unrealistic above 10 GeV. The FLUKA physics model is recommended above 3.5 GeV. For the ISABEL INC model, the correct upper limit is 1000 MeV (or 1000 MeV per nucleon for composite particles), although the model may execute above these limits. See the discussion of the **FLENB** input parameters below.

SWTM 0 ⇒ low-energy particles are written to file NEUTP unmodified;
> 0 ⇒ a roulette scheme is used for any particle with weight WT < SWTM.

The *default is 1.*; negative values are an error condition. If the particle weight WT < SWTM, the particle is killed with probability (1-WT/SWTM); otherwise, it is kept and given the weight SWTM. This option may be used to reduce the number of particles placed on the NEUTP file for subsequent MCNP tracking, while keeping the sampling frequency of high energy collisions large

WTPI The minimum weight for pions. The *default is 1.*; 0. or negative takes the default. If WTPI < WTMU, WTPI is set equal to WTMU. If the pion weight falls below WTPI, decay is allowed only by an analog process.

WTMU The minimum weight for muons produced by pion decay. The *default is 1.* and zero or negative takes the default. If WTMU equals 1., or if the pion weight is less than WTMU, pion decay is described by an essentially analog process. If WTMU < 1., more than one muon track may be produced per pion decay; on the average, 1/WTMU tracks for the decay of a weight 1. pion will be created.

Record type 8 List-directed with 2 items. For each medium M = 1,...,MXMAT, include one type 8 record followed by one or more type 9 records as needed. These records are absent if MXMAT = 0, a pure void problem.

DENH(M) Hydrogen (^{1}H) density in medium M, atoms/cubic Angstrom; the default is 0. This method of specifying hydrogen density is now **optional.** Hydrogen may

now be specified in the same fashion as any other isotope on record typ 9, in which case, DEHN should not be specified.

NEL(M) The number of nuclides or elements (other than ^{1}H if DENH is specified) in medium M. There is no default and the maximum is 100.

Record type 9 List-directed with 3 items. One type 9 record appears for each L, L=1,NEL(M).

ZZ(L,M) The charge number of the Lth nuclide or element in the Mth medium (no default).

A(L,M) The mass number of the Lth nuclide in the Mth medium; *the default is 0).* A naturally occurring element is specified by A = 0, or not entered at all. For example, "26,0," and "26,," will both indicate natural Fe. An element specified in this manner is expanded into its component isotopes and the atomic density is distributed by the naturally occurring atom fractions for the elements. Thus, if a natural element contains only one isotope, A need not be specified. **Warning:** this is the *mass number*, not the atomic weight; a non-integral value will cause errors.

DEN(L,M) The atom density (atoms per cubic Angstrom or barn-cm^2) of the Lth nuclide or element in the Mth medium (no default); it must be greater than 0.

Record types 1 through 9 are be followed, in order, by the following blocks of data:

- MCNP Geometry Records
- Other MCNP-type Records
- Source Specification Records

IV. MCNP Geometry Records

Warning: since LAHET uses "list-directed input" , the slash "/" may not be used on any MCNP geometry record *except* where it is a part of the surface type designator. The geometry input for the current operational version of LAHET is described in the older MCNP manual[12]. All features of the MCNP geometry capability are included in LAHET at the level of MCNP version 3A. The structure of the geometry input is as follows:

cell records
one blank line
surface records
one blank line
other MCNP-type records (see below)
one blank line.

The maximum number of cells or surfaces that may be input is no longer limited. *Note:* the material densities on the MCNP cell cards are *not* used by LAHET; the atom densities are taken from the type 9 records described above.

V. Other MCNP-type Records

TRn O_1 O_2 O_3 B_1 B_2 B_3 B_4 B_5 B_6 B_7 B_8 B_9 M
MCNP coordinate transformation record.

PRINT (No entries)
The presence of the PRINT record turns on the full printout of the MCNP geometry.

IN I_1 I_2 ... I_n
The IN input record represents true cell importances for the transport of nucleons, pions, and ions; I_i is the importance in cell i and may take on any positive real value. A zero importance cell still represents an external void. For information on variance reduction using cell-defined importances, see MCNP documentation; for impact on aspects of LAHET calculations, see reference [3].

IMU J_1 J_2 ... J_n
This record permits the (optional) input of a different set of importances J_i for muons when executing a coupled nucleon-pion-muon problem (NBERTP = -1). The use of the IMU record applies only when $I_i \neq J_i$ in one or more cells; in the absence of an IMU record, $I_i = J_i$ for $i = 1, ..., n$.

EMIN $EMIN_1$ ... $EMIN_{22}$
Energy cutoffs for all particle types; may be used to override default values for trackable particle types.

TRAN $ITRANS_1$ ... $ITRANS_{22}$
For each particle type, 1 indicates that the particle will be transported; 0 indicates that the particle type will not be transported if produced. Photons, electrons, positrons and neutrinos are *never* transported in LAHET3.

LSC *NSTRAG NSPRED NLRNGE SPRLM1 SPRLM2*

NSTRAG 0 ⇒ *no* range or energy straggling;
1 ⇒ Gaussian range straggling for charged particles *(default)*;
2 ⇒ energy straggling for charged particles.

Energy straggling is the most accurate method, but range straggling is appropriate for thick cells and is faster.

NSPRED 0 ⇒ multiple Coulomb scattering neglected;
1 ⇒ multiple scattering for primary charged particles only *(default)*;
2 ⇒ multiple scattering for *all* charged particles.

NLRNGE 0 ⇒ do *not* print range tables;
1 ⇒ print range tables.

SPRLM1 Fraction of charged particle range for nominal step size *(default is 0.1)*.

SPRLM2 Minimum charged particle step size *(default is 0.1 cm)*.

LCA IELAS IPREQ IEXISA ICHOIC JCOUL NEXITE NPIDK NOACT

IELAS 0 ⇒ no nucleon elastic scattering;
1 ⇒ elastic scattering for neutrons only;
2 ⇒ elastic scattering for neutrons and protons *(default)*.
3 ⇒ elastic scattering for all particles for which the cross section is defined.

For a description, see references [13],[14]. In the present release, elastic scattering is not available for ions.

IPREQ 0 ⇒ no preequilibrium model will be used *(default)*;
1 ⇒ use preequilibrium model after intranuclear cascade[15];
2 ⇒ use IPREQ =1 and IPREQ = 3 randomly, with an energy-dependent probability that goes to IPREQ = 3 at low incident energies and to IPREQ = 1 at high incident energies;
3 ⇒ use preequilibrium model *instead* of the intranuclear cascade.

Options IPREQ = 2 and IPREQ = 3 apply only when using the Bertini intranuclear cascade model (IEXISA = 0); when using the ISABEL model, these options default to IPREQ = 1. *Warning: options IPREQ = 2 or 3 have not been tested for consistency with new features introduced in LAHET3.* In addition, the preequilibrium model is applied only for incident nucleons in the present version.

IEXISA 0 ⇒ do NOT use ISABEL intranuclear cascade model for any particles;
1 ⇒ use Bertini model for nucleons and pions, with ISABEL model for other particle types *(default)*;
2 ⇒ use ISABEL model for all incident particle types.

The ISABEL intranuclear cascade model requires a much greater execution time. In addition, incident energies should be less than 1 GeV, or 1 GeV per nucleon for composite particles (although it may execute at higher energies). See references [16], [17], and [18].

ICHOIC A composite of four integers in the form *ijkl* which define the options for the ISABEL intranuclear cascade model.

$i = 0$ ⇒ use partial Pauli blocking *(default)*;
$= +1$ ⇒ use total Pauli blocking;
$=$ -1 ⇒ no Pauli blocking (not recommended for anything).
The ISABEL code input variable IPAULI $= i + 1$.

$j = 0$ ⇒ no interaction between particles already excited above the Fermi sea *(default)*;
> 0, the number of time steps to elapse between such "CAS-CAS" interactions.
The corresponding ISABEL code input variable is NTDEL, with default 3.

$k = 0 \Rightarrow$ Myer's density prescription with 8 steps;
$= 1 \Rightarrow$ original (isobar) density prescription with 8 steps;
$= 2 \Rightarrow$ Krappe's folded-Yukawa prescription for radial density in 16 steps, with a local density approximation to the Thomas-Fermi distribution for the (sharp cutoff) momentum distribution *(default)*;
$= 3 \Rightarrow$ the same as 0, but using the (larger) nuclear radius of the Bertini model;
$= 4 \Rightarrow$ the same as 1, but using the (larger) nuclear radius of the Bertini model;
$= 5 \Rightarrow$ the same as 2, but using the (larger) nuclear radius of the Bertini model.
The corresponding ISABEL code input variable is IDEN, with default also 2.

$l = 1 \Rightarrow$ reflection and refraction at the nuclear surface, but no escape cutoff for isobars;
$= 2 \Rightarrow$ reflection and refraction at the nuclear surface, with escape cutoff for isobars;
$= 3 \Rightarrow$ no reflection or refraction, with escape cutoff for isobars *(default)*;
$= 4 \Rightarrow$ the same as 1, but using a 25 MeV potential well for pions;
$= 5 \Rightarrow$ the same as 2, but using a 25 MeV potential well for pions;
$= 6 \Rightarrow$ the same as 3, but using a 25 MeV potential well for pions.
The corresponding input variable for the ISABEL code is MODEL $= l + 70$.

The default for ICHOIC is 23 (i.e., 0023); the defaults recommended for the ISABEL code would be represented by ICHOIC = 323. *Not all the options for the ISABEL intranuclear cascade model have been thoroughly tested.*

JCOUL 1 $\Rightarrow$ use Coulomb barrier on incident charged particle interactions *(default)*;
0 $\Rightarrow$ no Coulomb barrier for incident charged particles.

Applies only when $MODEXS \neq 0$ (i.e., the old cross section definition). The methodology is described in reference [19].

NEXITE 1 $\Rightarrow$ subtract nuclear recoil energy to obtain nuclear excitation energy *(default)*;
0 $\Rightarrow$ do not subtract nuclear recoil energy.

See reference [20] for a discussion.

NPIDK 1 $\Rightarrow$ force $\pi^-$to terminate by decay at the pion cutoff energy;
0 $\Rightarrow$ force $\pi^-$to interact by nuclear capture (intranuclear cascade) when cutoff is reached *(default)*.

The capture probability for any isotope in a material is proportional to the product of the number fraction and the charge of the isotope. However, capture on ^{1}H leads to decay rather than interaction.

NOACT 2 $\Rightarrow$ transport primary source particles without nonelastic reactions;
1 $\Rightarrow$ do NOT turn off nonelastic reactions *(default)*;
0 $\Rightarrow$ turn off all nonelastic reactions.

The use of this option is intended as a diagnostic tool, allowing other processes to be more easily observed.

LCB FLENB$_1$ *FLENB*$_2$ *FLENB*$_3$ *FLENB*$_4$ *FLENB*$_5$ *FLENB*$_6$ *CTOFE FLIM*0

FLENB$_1$, *FLENB*$_2$ For *nucleons,* the Bertini INC will be used below FLENB$_1$ while above FLENB$_2$ the FLUKA high-energy generator[5] will be used. The probability for selecting the interaction model is interpolated linearly with incident energy between these limits. *The defaults are 3490 MeV.* If FLENB$_1$ = FLENB$_2$, the transition between models is made at that unique energy; the ability to "phase in" the transition between models over an energy range is largely for "cosmetic" purposes. The *lower* limit (incident momentum) for the FLUKA model is 500 MeV/c. For nucleons, the BERTINI model switches to a scaling procedure above 3.495 GeV, wherein results are scaled from an interaction at 3.495 GeV. Although both models will execute to arbitrarily high energies, a plausible upper limit for the Bertini scaling law is 10 GeV.

FLENB$_3$, *FLENB*$_4$ For *pions,* these input parameters act as the above. *The defaults are 2490 MeV.* Note that for pions, the Bertini model switches to the scaling law method above 2.495 GeV.

FLENB$_5$, *FLENB*$_6$ These input parameters act like the pairs described above, but define the transition to the ISABEL INC below FLENB$_5$ to one of the higher energy models above FLENB$_6$, as appropriate for particle type and energy range. *The defaults are 800 MeV.* For IEXISA = 2, it applies to all particle types; for IEXISA = 1, it applies to all *except* nucleons and pions; for IEXISA = 0, it is immaterial. Consider the following example:

```
lcb    3000 3000 2000 2000 1000 1000
```

For $IEXISA = 1$, the default, nucleons would switch to the Bertini model from the FLUKA model below 3 GeV and pions would switch below 2 GeV. Kaons and antinucleons would switch to the ISABEL model from the FLUKA model below 1 GeV. (Ions use only the ISABEL model and muons have no nuclear interactions in LAHET). For IEXISA = 2, nucleons and pions would also switch to the ISABEL model below 1 GeV. Note that the nominal upper energy limit for the ISABEL model is about 1 GeV/nucleon; it may actually execute at higher energies without "crashing", but with diminished validity.

CTOFE The cutoff energy (MeV) for particle escape during the intranuclear cascade *when using the Bertini model.* The cutoff energy prevents low energy nucleons from escaping the nucleus during the intranuclear cascade; for protons, the actual cutoff is the *maximum* of CTOFE and a Coulomb barrier. For CTOFE ≥ 0, CTOFE will be used as the cutoff energy. For CTOFE < 0, a *random* cutoff energy, uniformly distributed from zero to twice the mean binding energy of a nucleon, will be sampled for each projectile-target interaction and separately for neutrons and protons; in this case, the Coulomb barrier for protons is also randomized. *The randomized cutoff energy is the default procedure;* i. e. CTOFE = -1 is the default value. For the ISABEL INC, the randomized cutoff energy is always used.

FLIM0 The maximum correction allowed for mass-energy balancing in the cascade stage, used with NOBAL = 1 and NOBAL = 3. For FLIM0 > 0, kinetic energies of secondary particles will be reduced by no more than a fraction of FLIM0 in attempting to obtain a non-negative excitation of the residual nucleus and a consistent mass-energy balance; a cascade will be resampled if the correction exceeds FLIM0. For FLIM0 = 0, no correction will be attempted and a cascade will be resampled if a negative excitation is produced. For FLIM0 < 0 *(default)*, a procedure is used in which the maximum correction is 0.02 for incident energy above 250 MeV, 0.05 for incident energy below 100 MeV, and is set equal to 5/(incident energy) between those limits.

LEA IPHT ICC NOBALC NOBALE IFBRK ILVDEN IEVAP NOFIS

IPHT 0 $\Rightarrow$ do NOT generated photons in the evaporation stage;
1 $\Rightarrow$ generate de-excitation photons.

The *default is IPHT = 1.*

ICC ICC defines the level of physics to be applied. Values of 0 through 4 are allowed. The definitions of the physics options defined by ICC are discussed below. The *default is ICC = 4.*

- For ICC = 1, the nuclear energy levels specified in the data library are used. The continuum is assumed to begin above the highest specified level. However, all transitions, whether continuum-to-continuum, continuum-to-level, or level-to-level, are assumed to be E1 transitions.
- When ICC = 2, the model employed is really a hybrid between models 1 and 3. The nuclear levels, and their spins and parities, are obtained from the data library. The continuum begins above the highest specified level. However, all levels above the lowest that has unknown spin or parity are considered to also have unknown spin. All transitions within or from the continuum, or that involve a level with unknown spin, are treated as E1 transitions as in model 1. All transitions involving only states of known spin and parity utilize the Weisskopf single particle transition model as in option 4.

- The ICC = 3 option gives the full model as described in section 5.1, with the exception that any experimental branching ratios are ignored and a pure model calculation is performed for the transition probabilities using the Weisskopf single particle transition estimates.
- With ICC = 4, the full procedure described in section 5.1 is employed, including the use of library-specified branching ratios when available.

NOBALC 0 ⇒ use mass-energy balancing in the cascade stage;
1 ⇒ turn off mass-energy balancing in the cascade stage.

The *default is NOBALC = 1.* A forced energy balance may distort the intent of any intranuclear cascade model; the user should explore the effect of energy balancing, utilizing HTAPE with option 7. Energy balancing for the intranuclear cascade is controlled by input parameter FLIM0 below. NOBALC *applies only to Bertini model and ISABEL interactions.*

NOBALE 0 ⇒ use mass-energy balancing in the evaporation stage;
1 ⇒ turn off mass-energy balancing in the evaporation stage.

The *default is NOBALE = 0.*

IFBRK 1 ⇒ use Fermi breakup model for A $\leq$ 13 and for 14 $\leq$ A $\leq$ 20 with excitation below 44 MeV *(default)*;
0 ⇒ use Fermi breakup model only for A $\leq$ 5.

ILVDEN -1 ⇒ use original HETC level density formulation;
0 ⇒ use Gilbert-Cameron-Cook-Ignatyuk level density model *(default)* [15];
1 ⇒ use the Jülich level density parameterization as a function of mass number [21].

IEVAP 0 ⇒ the RAL evaporation-fission model will be used *(default)* [22];
1 ⇒ the ORNL evaporation-fission model will be used [23].

The ORNL model allows fission only for isotopes with Z $\geq$ 91.

NOFIS 1 ⇒ allow fission *(default)*;
0 ⇒ suppress fission.

LEB YZERE BZERE YZERO BZERO

YZERE The Y0 parameter in the level density formula for Z $\leq$ 70. The default is 1.5; zero or negative is an error condition. For target nuclei with Z $\leq$ 70, the parameters BZERE and YZERE are used to compute level densities; the default values are those used in LAHET before installation of the ORNL fission model. For target nuclei with Z $\geq$ 71, the BZERO and YZERO parameters are used to compute level densities for the target nucleus and the fission fragments. *Applies only for ILVDEN = -1.*

BZERE The B0 parameter in the level density formula for Z $\leq$ 70. The default is 8.0; zero or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.*

YZERO The Y0 parameter in the level density formula for Z $\geq$ 71 and all fission fragments. The default is 1.5; zero or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.*

BZERO The B0 parameter in the level density formula for Z $\geq$ 71 and all fission fragments. The default is 14.0 for IEVAP = 0 and is 10.0 for IEVAP = 1; 0 or negative is an error condition (see YZERE above). *Applies only for ILVDEN = -1.*

VI. Source Specification Records

To specify one of the allowed default source options, at least the following record must be supplied. It is in list-directed format with up to 10 data items.

ISOPT -1 $\Rightarrow$ An *isotropic* point source in the (x,y)-plane;
0 $\Rightarrow$ A parallel beam uniformly distributed over an ellipse (default);
1 $\Rightarrow$ A parallel beam with parabolic density over an ellipse;
2 $\Rightarrow$ A parallel beam with Gaussian density over an ellipse;
3 $\Rightarrow$ A parallel beam elliptical ring source with user-supplied density distribution;
4 $\Rightarrow$ A parallel beam uniformly distributed in a rectangle;
5 $\Rightarrow$ Incoming isotropic source on a sphere (or hemisphere);
9 $\Rightarrow$ The same as ISOPT = -1 with input energy distribution;
10 $\Rightarrow$ The same as ISOPT = 0 with input energy distribution;
11 $\Rightarrow$ The same as ISOPT = 1 with input energy distribution;
12 $\Rightarrow$ The same as ISOPT = 2 with input energy distribution;
13 $\Rightarrow$ The same as ISOPT = 3 with input energy distribution;
14 $\Rightarrow$ The same as ISOPT = 4 with input energy distribution;
15 $\Rightarrow$ The same as ISOPT = 5 with input energy distribution.

E0 The source energy in MeV; the default is 800 MeV. For the parallel beam sources, the *sign* applied to E0 is relevant. If a negative value for E0 is entered, the source particles are emitted in the negative z-direction and the absolute value of E0 is used as the source energy; otherwise, the source is emitted in the positive z-direction. E0 applies only to ISOPT = -1,...,5.

TIP0 The source particle type in floating point from Table 2. The default is 0.0 (proton). Nucleons and charged pions will interact when transported using either intranuclear cascade model. Muons will slow down and decay without nuclear interaction. The ion types 7. through 10. will interact using the ISABEL model, but will only slow down otherwise. Antinucleons and kaons may be used for a cross section interaction calculation (N1COL=-1) only, since provision for transporting kaons has not yet been implemented. Photons and π^0's may not be input as source particles.

Z0 The starting z-coordinate for the source (the default is 0.0). For ISOPT = 5 or 15, Z0 is the z-coordinate of the center of the source sphere. A value of Z0 should be selected such that the source *does not coincide exactly with a plane* separating two cells; a very small shift in the beam direction will suffice. If the source is coincident exactly with a plane separating an importance 1 cell from an importance 0 cell, histories will be lost since some source particles will be born in an external void region. (A warning of this condition is printed out in file OUTH). In other cases, tracking errors may occur.

A0 The semi-major axis parameter. The default is 0.0; a value of 0.0 will produce a "pencil beam" source. For ISOPT = 4 or 14, A0 is the rectangular half-length along the x'-axis. For ISOPT = 5 or 15, A0 is the radius of the source sphere. For ISOPT = -1 or 9, A0 is unused. To understand the option-dependent definition of A0, the user *must* read the following section.

B0 The semi-minor axis parameter. The default is A0; if B0 = A0, a circular (or square) source will be produced. For ISOPT = 4 or 14, B0 is the rectangular half-length along the y'-axis. *NOTE*: for the *elliptical* sources (ISOPT = 0, 1, 2, 3, 10, 11, 12, or 13) B0 $\leq$ A0 is *required*. For ISOPT = -1 or 9, B0 is unused. For ISOPT = 5 or 15, B0 is unused. To understand the option-dependent definition of B0, the user *must* read the following section.

CUTS The cutoff parameter used with ISOPT = 1, 2, 11, or 12. The default is 1.0 for ISOPT = 1 or 11 and is 3.717 for ISOPT = 2 or 12; in either case, zero takes the default. CUTS is not used for ISOPT = -1, 0, 3, 4, 9, 10, 13, or 14. For ISOPT = 1 or 11, CUTS should be between 0 and 1; CUTS = 1.0 is the same as no cutoff at all. For ISOPT = 2 or 12, any positive value is allowed. For ISOPT = -1 or 9, CUTS is unused. For ISOPT = 5 or 15, CUTS is unused. To understand the use of CUTS, the user is referred to the original documentation[2]

SMU The cosine of rotation of the source ellipse or rectangle (the default is 0.0). SMU is immaterial for A0 = B0 unless ISOPT = 4 or 14). To fully understand the definition and use of SMU, see [2]. Note that SMU = 0.0 implies no transformation at all. For ISOPT = -1 or 9, SMU is unused. For ISOPT = 5 or 15, SMU has a special meaning:

- SMU = 0 puts there source uniformly over the entire sphere;
- SMU > 0 puts the source only on the +Z hemisphere;
- SMU < 0 puts the source only on the -Z hemisphere.

X0 The x-coordinate for the center of the source distribution (the default is 0.0). For ISOPT = 5 or 15, X0 is the x-coordinate of the center of the source sphere.

Y0 The y-coordinate for the center of the source distribution (the default is 0.0). For ISOPT = 5 or 15, Y0 is the y-coordinate of the center of the source sphere.

For ISOPT = 3 or 13, the following two additional records must be supplied; each is in list-directed format and may contain up to 100 entries.

SRING2(I),I=1,NRING Ring boundary parameters for NRING elliptical rings in increasing order.

SPROB(I),I=1,NRING Ring probability values for NRING elliptical rings. They need not be normalized.

The items of the above two records must be in a one-to-one correspondence. The function of ISOPT = 3 or 13 is described below.

To specify a probability distribution for the source particle energy with ISOPT = 9 through 15, two records must be supplied which may have up to 200 entries.

ESRC(I),I=1,NEPRB Energy bin boundaries for NEPRB-1 energy bins, within each of which the source energy will be uniformly sampled.

EPRB(I),I=1,NEPRB Probability specification for sampling from the NEPRB-1 energy bins, in either of the two forms described below.

The EPRB array may be entered *either* as the unnormalized energy probability density value times the bin width for each energy bin *or* as the corresponding cumulative source energy distribution values. In either case, EPRB(1) *must be* 0. The cumulative distribution method is determined by the fact that the last EPRB entry must be *precisely unity*; consequently, when using the first method, the last EPRB entry must not be unity. As an example, consider the energy probability table entered as

```
100.,200.,400./
0.,6.,4./
```

In this case, the source energy bin from 100 MeV to 200 MeV will be sampled 60% of the time and the bin from 200 MeV to 400 MeV will be sampled 40% of the time. The same distribution entered using the cumulative density method would use the records

```
100.,200.,400./
0.,.6,1./
```

In either case, the probability density in the first bin is 0.006/MeV and in the second is 0.002/MeV.

If desired, the user may add a record after the above spatial source description to assign a time dependence to the source pulse. The source time record is list-directed with 4 data items and has the form "**ITOPT,TWIT,TPEAK,TSIG/**".

ITOPT -1 ⇒ Set the source time to TPEAK (default);
0 ⇒ Sample the source time from a uniform distribution of width TWIT centered at TPEAK.
1 ⇒ Sample the source time from a parabolic distribution of width TWIT centered at TPEAK.
2 ⇒ Sample the source time from a Gaussian distribution of standard deviation TSIG centered at TPEAK with width TWIT.
3 ⇒ Sample the source time from a user-input probability table.

TWIT The source pulse width in nanoseconds (the default is 0).

TPEAK The pulse center in nanoseconds (the default is 0).

TSIG The standard deviation of a Gaussian pulse (the default is TWIT/4).

The parameters TWIT and TPEAK are meaningful only for ITOPT = 0, 1, or 2; TSIG is meaningful only for ITOPT = 2. For ITOPT = 3, the following two records, with up to 200 entries each, must be supplied to give the source time probability distribution.

TSRC(I),I=1,NTPRB Time bin boundaries for NTPRB-1 time bins, within each of which the source time will be uniformly sampled.

TPRB(I),I=1,NTPRB Probability specification for sampling from the NTPRB-1 time bins.

The methods for entering (and sampling from) the TSRC and TPRB arrays is exactly the same as for the ESRC and EPRB arrays described above. TPRB(1) *must be* 0.

VII. Using MCNP with LAHET

MCNP Versions 4B and 4C[6] contain both

- all the coding and features of HMCNP4A;
- the new MCNP option to produce a "surface source write" WSSA file to be edited by HTAPE using the SSW output option.

With the new modification to the SSW option, MCNP contains all the features originally developed for HMCNP. To use old HMCNP input files with MCNP, remove the FILES and FU input records and use the SSR and SSW options as described below.

A NEUTP file written by LAHET3 may now contain both neutrons and photons as source particles for MCNP. The file is written in the format of an MCNP volume particle source RSSA file. By any method, change the name NEUTP to RSSA and use the SSR source option in MCNP.

For the new output file option, use the SSW output option in the INP file with the following form:

SSW S_1 S_2 ... S_n SYM=2

Do not define unit 70 on the FILES input record. The option "SYM=2" is new; it causes a surface crossing record to be written for a particle crossing in **either** direction across specified surface S_i. One way to input the WSSA file produced into HTAPE is to use the following syntax:

HTAPE HISTX=WSSA

HTAPE will determine the format of the input file from the header record.

VIII. Plotting Output from XSEX3

The source code for XSEX3 contains a plotting package using the LANL Common Graphics System; the latter is not generally available outside of Los Alamos National Laboratory. A new feature has been added for this release whereby a nonzero value for the input quantity KPLOT will cause the writing of a file XSTAL in the format of an MCNP MCTAL file. Plotting of XSTAL is performed by MCNP, using the execution option

```
mcnp z
```

followed by the instructions

```
rmctal xstal
nonorm
```

The latter is essential since the data are normalized in XSEX3.

When plotting XSEX3 output, the appropriate y-axis labels are "barns/MeV/steradian", "barns/MeV" or "barns/steradian". If the "yield" (multiplicity) option was used in XSEX3, the appropriate y-axis labels are "particles/MeV/steradian", *etc.* The energy axis may be either "energy (MeV)" or "momentum (MeV/c)" according to the XSEX3 option employed.

Each "case" in XSEX3 is expanded in the XSTAL file for each particle type produced. The tallies are identified by the numbering scheme **100(case number) + (particle type)**. The last in the sequence corresponds to the elastic scattering distribution of the incident particle.

Table 1: Cross section definition in LAHET3

Proton elastic

Energy range	A>: 2-3	A:4-8	A>8
E<3GeV	LAHET2.8	B&P	LAHET2.8
3GeV<E<30GeV	interpolated	interpolated	interpolated
E>30GeV	FLUKA96	FLUKA96	FLUKA96

Neutron elastic

Energy range	A = 2,3	A: 4-8	A > 8
E<20MeV	none	none	none
20 MeV<E<50MeV	EVAL	B&P	EVAL
50MeV<E<100MeV	interpolated	B&P	interpolated
100MeV<E<3GeV	LAHET2.8	B&P	LAHET2.8
3GeV<E<30GeV	interpolated	interpolated	interpolated
E>30GeV	FLUKA96	FLUKA96	FLUKA96

Proton reaction

Energy range	A=2	A: 3-9	A = 10,11	A: 12-210	A > 210
E<50MeV	FLUKA96	NASA (1)	FLUKA96	FLUKA96	NASA
50MeV<E<100MeV	FLUKA96	NASA (1)	FLUKA96	interpolated	NASA
100MeV<E<400MeV	FLUKA96	NASA (1)	FLUKA96	OM	NASA
400MeV<E<1GeV	FLUKA96	NASA (1)	FLUKA96	interpolated	NASA
1GeV<E<10GeV	FLUKA96	interpolated	FLUKA96	FLUKA96	interpolated
E>10GeV	FLUKA96	FLUKA96	FLUKA96	FLUKA96	FLUKA96

(1) A=3,Z=1 treated as A=3,Z=2

Neutron reaction

Energy range	A=2	A = 3,4	A: 6-8	A: 9-11	A: 12-210	A > 210
E<20MeV	none	none	none	none	none	none
20MeV<E<50MeV	EVAL	FLUKA96	B&P	EVAL	EVAL	EVAL
50MeV<E<80MeV	EVAL	FLUKA96	B&P	EVAL	EVAL	interpolated
80MeV<E<100MeV	EVAL	FLUKA96	B&P	interpolated	EVAL	interpolated
100MeV<E<150MeV	interpolated	FLUKA96	B&P	B&P	interpolated	FLUKA96
150MeV<E<300MeV	interpolated	FLUKA96	B&P	B&P	OM	FLUKA96
300MeV<E<400MeV	FLUKA96	FLUKA96	B&P	B&P	OM	FLUKA96
400MeV<E<1GeV	FLUKA96	FLUKA96	B&P	B&P	interpolated	FLUKA96
1GeV<E<10GeV	FLUKA96	FLUKA96	interpolated	interpolated	FLUKA96	FLUKA96
E>10GeV	FLUKA96	FLUKA96	FLUKA96	FLUKA96	FLUKA96	FLUKA96

Table 1 (cont.): Cross section definition in LAHET3

Pion elastic	
Energy range	**A>1**
E<40MeV	B&P
40MeV<E<51MeV	interpolated
E>51MeV	FLUKA96

Pion reaction	
Energy range	**A>1**
E<40MeV	B&P
40MeV<E<51MeV	interpolated
E>51MeV	FLUKA96

Kaon elastic	
Energy range	**A>1**
all E	FLUKA96

Kaon elastic	
Energy range	**A>1**
all E	FLUKA96

Antinucleon elastic	
Energy range	**A>1**
all E	FLUKA96

Antinucleon reaction	
Energy range	**A>1**
all E	FLUKA96

LAHET2.8:	reference [14]
OM:	additional optical model results as in reference [14]
B&P:	method of Barashenkov and Polanski, reference [11]
FLUKA96:	coding from FLUKA96, references [7],[11]
EVAL:	tabulation obtained from MCNP 150MeV neutron data libraries, reference [11]
NASA:	NASA formulation (Tripathi), reference [11]

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